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Effects of surface reconstruction on III–V semiconductor interface formation: The role of III/V composition

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Using molecular-beam epitaxy and *in situ* scanning tunneling microscopy, we demonstrate how different reconstructions associated with different III–V growth surfaces can create interfacial roughness, and that an understanding of this phenomenon can be used to control the roughness on the atomic scale. Specifically, the different compositions of a clean InAs(001)-(2×4) surface ($V/III=0.5$ ML/0.75 ML) and an Sb-terminated one ($\sim$1.7 ML/1 ML) cause the InSb-like interfacial surface to have a bilevel morphology. This surface roughness can be eliminated by depositing additional In to exactly compensate for the difference. It is likely that similar types of roughness occur in all heterostructures where the growth surface reconstruction changes at the interfaces, and that a similar procedure will be equally effective at reducing that roughness. © *1999 American Institute of Physics.* [S0003-6951(99)01112-2]

Fabrication of high-quality III–V semiconductor electronic devices requires precise control of epitaxial growth, usually on III–V(001) substrates. One of the most notable aspects of such substrate surfaces is the variety of reconstructions observed under different III/V flux ratios and substrate temperatures.[1] At least two distinctive features of these reconstructions could potentially affect epitaxial growth: (1) they are structurally anisotropic, a consequence of the tetrahedral bonding and the zinc-blende crystal structure; and (2) they occur with a wide range of III/V stoichiometries, both less than and greater than unity. There is theoretical[2,3] and experimental[4–7] evidence that the structural anisotropy does, in fact, affect nucleation and growth during both homo- and heteroepitaxy, in part by causing surface diffusion to be anisotropic. The structural anisotropy also plays an important role in compositional modulation and ordering in III–V alloys (such as GaInP).[8] The most obvious effect one would expect from a III/V ratio$\neq 1$ is intermixing at heterostructure interfaces, a phenomenon often observed but only recently correlated directly with surface reconstruction.[9]

The effects of surface reconstruction on epitaxy are not just an esoteric concern. It is well known that the interfacial disorder that may result, due to morphological roughness or intermixing, can cause observable effects on the properties of electronic and optical devices. Recent examples of such effects directly attributed to interface quality include an anisotropic reduction in mobility observed in InAs/GaInSb superlattices,[6] and a growth-temperature-dependent reduction in photoluminescence intensity in infrared laser structures.[10] Devices utilizing layers only a few monolayers thick, such as resonant tunneling diodes (RTDs), are expected to be particularly sensitive to these growth anomalies.[11,12] To date, discussion of reconstruction-induced surface and interfacial structures has been limited to their characterization. In this letter we demonstrate how an atomic-scale understanding of surface structure can actually be used to *control* the roughness at a III–V heterostructure interface, specifically, an interface where the growth surface reconstruction changes III/V composition.

The experiments were performed in an interconnected, multichamber ultra-high-vacuum facility that includes a III–V molecular-beam epitaxy (MBE) chamber equipped with reflection high-energy electron diffraction (RHEED) and an analysis chamber equipped with a scanning tunneling microscope (STM).[13] Samples were grown on InAs(001) wafers using ''cracked'' As_2 and Sb_2 sources. First, an undoped InAs buffer layer $\sim$0.5 μm thick was grown at 1 ML/s using an As:In beam equivalent pressure ratio of 5:1 and 30 s growth interrupts every 90 s. The growth temperature of this layer was approximately equal to the congruent sublimation temperature of InAs, estimated to be 470 °C. At the end of this growth, a 10 min interrupt was performed during which the As_2 flux was reduced while maintaining a sharp (2×4) RHEED pattern. We have shown that this procedure produces a surface with a nearly ideal, island-free terrace-plus-step morphology.[14] Upon completion of the buffer layer, the samples were then cooled to $\sim$400 °C and an Sb/InAs interface was created using migration-enhanced epitaxy (MEE): an additional In layer was deposited first (with no As_2 flux), followed by 2 s of Sb_2 (with no In flux). The samples were then cooled rapidly and transferred *in vacuo* to the STM chamber. All STM images shown were acquired at room temperature with sample biases between -1.5 and -2.7 V and tunneling currents of 30–200 pA.

A STM image of the InAs buffer layer surface is shown in Fig. 1(a). The surface is composed of well-ordered (2×4)-reconstructed terraces separated by monolayer-height (0.3 nm) steps. Atomic-resolution images (not shown) are similar in appearance to those previously published for InAs

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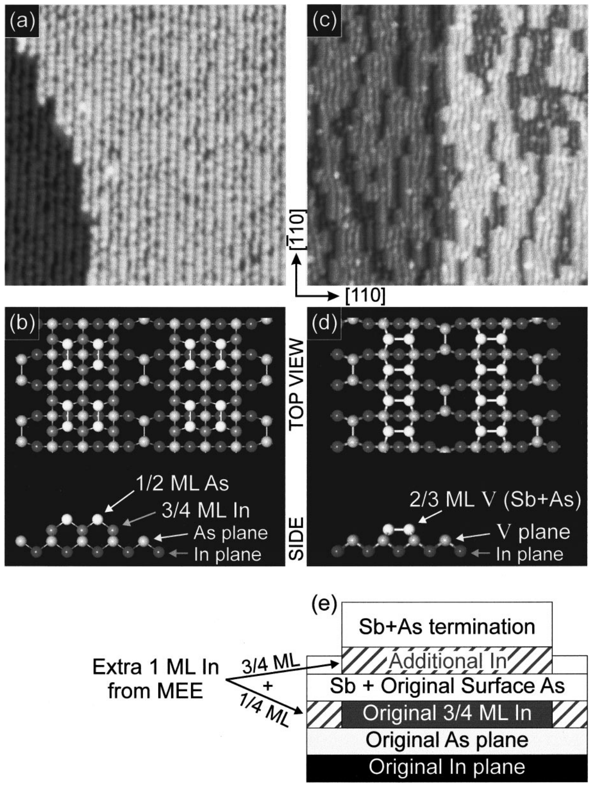

FIG. 1. (a) Filled-state STM image of a clean InAs(001)-(2×4) surface ($50\,\text{nm}\times50\,\text{nm}$). A monolayer-height (0.3 nm) step is visible. (b) The $\beta2(2\times4)$ model for the surface reconstruction. The rows observed in the STM image are associated with the rows of As dimer pairs in the model. (c) A similar area on the surface at the same magnification after depositing 1 ML In and exposing to 2 s of Sb_2 at ~400 °C. A substrate terrace edge runs up the middle of the image. (d) A model of the idealized surface structure after Sb exposure. The meandering rows seen in the STM image correspond to the top-most rows of group V surface dimers. (e) A schematic illustration of the proposed surface composition associated with the surface morphology observed in (c).

and GaAs(001)-(2×4), consistent with the generally accepted $\beta2(2\times4)$ model for the reconstruction.[1] In this model, illustrated in Fig. 1(b), the top III–V layer is nonstoichiometric, with only $\frac{1}{2}$ ML As and $\frac{3}{4}$ ML In. The surface is terminated by $[\bar{1}10]$-oriented rows of As dimer pairs (it is these rows that are visible in the STM image shown), separated by a row of single As dimers one III–V layer below.

We have recently been studying the evolution of the surfaces and interfaces during the growth of InAs/AlSb/InAs RTDs, and have observed that the initial Sb-on-InAs interface—formed in preparation for the growth of the critical AlSb barrier—is accompanied by a dramatic change in surface morphology.[14] When the nearly ideal InAs(001)-(2×4) surface is exposed to Sb_2, a bilayer surface is produced with 1–10 nm wide, one layer deep (0.3 nm) vacancy islands covering approximately 25% of the surface (independent of the length of the exposure). A STM image of one such surface is shown in Fig. 1(c), created using the MEE procedure described above with 1 ML of In deposited followed by a 2 s exposure to Sb_2. During RTD fabrication this procedure is used to create InSb-like interfacial bonds, which generally lead to more desirable device properties than III–As-like bonds.[10,15,16] When this surface is created, the RHEED pattern changes from (2×4) to (1×3), and the rows observed in the STM images change from the regular $\times4$ period to a meandering $\times3$ separation. At higher magnification (not shown), the meandering rows appear to be composed of single dimers with a bond axis parallel to [110] (perpendicular to the 2×4 surface dimer orientation).

In general, the InSb-like surface layer on InAs(001) has a very similar appearance to (1×3)-like reconstructions observed on InSb,[17] AlSb,[18] and GaSb(001).[19] Although the structure of this reconstruction has not been definitively determined (e.g., by atomic-resolution experimental and first-principles theoretical techniques), based on our images and recent studies of analogous GaSb reconstructions,[19–21] we believe this ''(1×3)'' surface actually has a disordered $c(2\times6)$ structure, with a composition similar to that shown in Fig. 1(d). In contrast to the $\beta2(2\times4)$ reconstruction, where the surface has <1 ML of both III and V atoms, this V-rich structure consists of a *full* plane of In terminated by a double-layer of group V atoms. If the surface dimer rows were free of kinks and defects, the group V coverage would be $1\frac{2}{3}$ ML. Note that although there is evidence that exposing the InAs(001)-(2×4) surface to Sb induces an Sb-for-As exchange reaction,[22] this reaction may be suppressed by the MEE procedure employed here. We suspect that in our case the surface group V double layer consists of a mixture of Sb and remnant As.

Because the Sb/InAs surface represents the first in a series of increasingly rough interfaces in our RTD structure,[14] smoothing this surface is the first step to improving the interfaces throughout the device. We have determined that the Sb-induced surface roughening is a direct consequence of the different III/V compositions in the InSb-like $c(2\times6)$ vs InAs(001)-(2×4) reconstructions, as shown schematically in Fig. 1(e). Assuming the clean InAs surface has only $\frac{3}{4}$ ML of In, of the additional 1 ML of In deposited during the MEE procedure, $\frac{1}{4}$ ML is required to form the complete In plane that becomes the base for the $c(2\times6)$ reconstruction. Therefore, only $\frac{3}{4}$ ML In remains for the top layer of InSb-like islands on the surface (or, equivalently, the top layer is left with $\frac{1}{4}$ ML of vacancies). This origin for the islands is confirmed by the dependence of the island/vacancy coverage on the amount of In deposited during the interface formation, as illustrated in Fig. 2. If only $\frac{3}{4}$ ML of In is deposited during the MEE step—leaving only $\frac{1}{2}$ ML for the overlayer islands—each substrate terrace is divided equally between the two InSb-like levels after Sb_2 exposure, as expected [Fig. 2(a)]. For comparison, a comparable image of a surface made with the original MEE procedure is also shown [Fig. 2(b)], quantitatively showing the 25%/75% bifurcation on each terrace. The final extension of this procedure is to deposit the ''correct'' amount of In ($1\frac{1}{4}$ ML) needed to compensate for the different compositions of the two reconstructions. The resulting ''optimized'' interface is almost perfectly flat, as shown in Fig. 2(c), with over 95% of each terrace on a single level.[23] The fact that the island coverage correlates with the In coverage exactly as expected based on the reconstructions shown in Fig. 1 is also strong evidence that these models, as assumed, are essentially correct.

Given that the formation of the bilevel Sb/InAs surface involves rearrangement within two III–V surface layers, one might expect that the resulting vacancy islands could be ''annealed out'' by longer growth interrupts under Sb_2. Surpris-

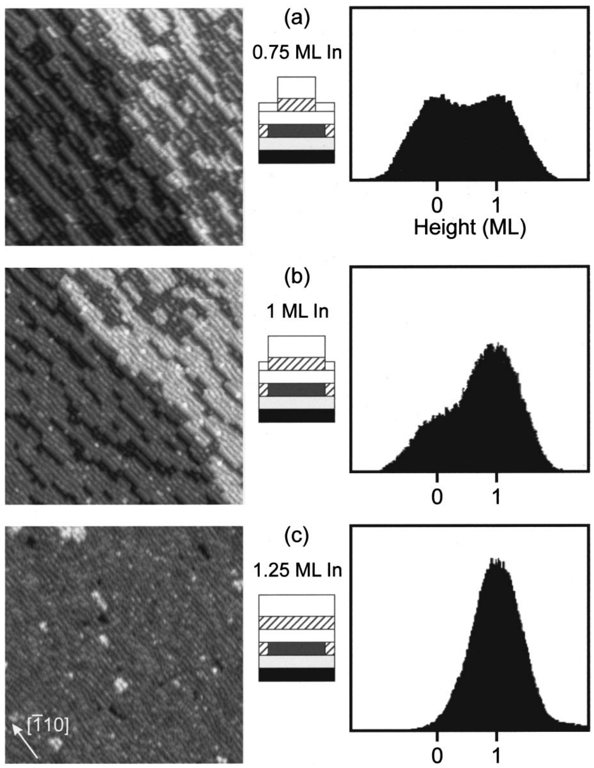

FIG. 2. (a) Filled-state STM images, 60 nm×60 nm, of an InAs(001) surface after depositing different amounts of In and then exposing to 2 s of Sb_2 at ~400 °C: (a) 0.75 ML In, (b) 1 ML In, and (c) 1.25 ML In. The histograms show the height distributions on each surface (within one substrate terrace). The histograms in (a) and (b) have a bimodal height distribution corresponding to 50% and 25% vacancy coverage, respectively. In (c) 95% of the surface is at the main terrace level. A schematic of the surface layer composition is shown for each case, shaded identically to Fig. 1(e).

ingly, *they cannot*. Although the islands do coarsen somewhat with longer interrupts, the vacancy coverage is unchanged.[14] Even a long (10 min) interrupt at a higher temperature (~500 °C) does not smooth the surface. Rather, a highly anisotropic striated surface morphology develops, indicating the *equilibrium* Sb/InAs structure involves a more complex multilayer reconstruction of the surface[24] (one that is probably undesirable from the standpoint of achieving abrupt interfaces). Within our experience, the islands can only be eliminated by depositing additional In with MEE.

In conclusion, we have shown that different surface reconstructions across a III–V heterointerface can create morphological roughness, and that an understanding of this phenomenon can be used to control the roughness on the atomic scale. Specifically, the different III/V compositions on clean InAs(001)-(2×4) versus an Sb-terminated surface (created upon the formation of InSb-like interfacial bonds) split the surface into two levels, but this bifurcation can be eliminated by adding the appropriate amount of In to the interface to compensate for the difference. Because the $\beta 2(2\times4)$ reconstruction is common to all III–As(001) growth surfaces, and the III–Sb surfaces all appear to share a similar Sb-rich structure, we expect this procedure to be widely applicable to III–Sb/III–As(001) interfaces. Moreover, it is likely that similar types of roughness occur in *all* heterostructures where the growth surface reconstruction changes at the interfaces, and that similar growth techniques will be equally effective at reducing that roughness.

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